

## Appendix A: Additional tables

**Table A.1.** Observed transitions and line parameters derived from Gaussian fits. Rest frequencies and spectroscopic data are taken from the MADEX catalogue (Cernicharo 2012).

Transition	Frequency (MHz)	$E_{up}$ (K)	$A_{ul}$ ( $s^{-1}$ )	$\int T_A^* dv$ (mK km s $^{-1}$ )	$V_{LSR}$ (km s $^{-1}$ )	$\Delta v$ (km s $^{-1}$ )	$T_A^*$ (mK)
<b>NCO (<math>^2\Pi_{3/2}</math>)</b>							
$J = 7/2 - 5/2$ $F = 9/2 - 7/2$ $e$	81404.300	6.6	$9.19 \cdot 10^{-7}$	3.6(9)	5.32( 4)	0.42(10)	8.0
$J = 7/2 - 5/2$ $F = 9/2 - 7/2$ $f$	81404.813	6.6	$9.19 \cdot 10^{-7}$	4.1(9)	5.41( 3)	0.42( 7)	9.0
$J = 7/2 - 5/2$ $F = 7/2 - 5/2$ $e$	81413.120	6.6	$8.44 \cdot 10^{-7}$	2.1(9)	5.45( 4)	0.34(10)	5.9
$J = 7/2 - 5/2$ $F = 7/2 - 5/2$ $f$	81413.573	6.6	$8.44 \cdot 10^{-7}$	3.2(9)	5.26( 4)	0.45(10)	6.6
$J = 7/2 - 5/2$ $F = 5/2 - 3/2$ $e$	81418.385	6.6	$8.17 \cdot 10^{-7}$	2.9(9)	5.24( 6)	0.44(11)	6.2
$J = 7/2 - 5/2$ $F = 5/2 - 3/2$ $f$	81418.884	6.6	$8.17 \cdot 10^{-7}$	1.6(9)	5.43( 5)	0.27(17)	5.4
$J = 9/2 - 7/2$ $F = 11/2 - 9/2$ $e$	104665.278	11.7	$2.19 \cdot 10^{-6}$	5.0(9)	5.45( 5)	0.55(10)	8.6
$J = 9/2 - 7/2$ $F = 11/2 - 9/2$ $f$	104666.098	11.7	$2.19 \cdot 10^{-6}$	5.4(9)	5.43( 4)	0.55( 7)	9.1
$J = 9/2 - 7/2$ $F = 9/2 - 7/2$ $e$	104670.139	11.7	$2.08 \cdot 10^{-6}$	3.6(9)	5.36( 4)	0.45(11)	7.6
$J = 9/2 - 7/2$ $F = 9/2 - 7/2$ $f$	104670.905	11.7	$2.08 \cdot 10^{-6}$	3.9(9)	5.35( 3)	0.37( 8)	9.9
$J = 9/2 - 7/2$ $F = 7/2 - 5/2$ $e$	104673.371	11.7	$2.05 \cdot 10^{-6}$	1.6(9)	5.26( 4)	0.22( 7)	7.1
$J = 9/2 - 7/2$ $F = 7/2 - 5/2$ $f$	104674.173	11.7	$2.05 \cdot 10^{-6}$	2.9(9)	5.32( 4)	0.35( 8)	7.8
<b>H<sub>2</sub>NCO<sup>+</sup></b>							
$4_{1,4} - 3_{1,3}$	80246.376	8.7	$4.28 \cdot 10^{-5}$	2.0(5)	5.02( 1)	0.18(60)	10.4
$4_{0,4} - 3_{0,3}$	80906.926	9.7	$4.67 \cdot 10^{-5}$	2.8(5)	5.32( 5)	0.53( 9)	4.9
$4_{1,3} - 3_{1,2}$	81565.636	8.8	$4.49 \cdot 10^{-5}$	4.9(9)	5.16( 5)	0.63(10)	7.3
$5_{1,5} - 4_{1,4}$	100306.949	13.5	$8.74 \cdot 10^{-5}$	5.0(5)	5.37( 3)	0.53( 5)	8.9
$5_{0,5} - 4_{0,4}$	101131.130	14.6	$9.33 \cdot 10^{-5}$	3.8(9)	5.45( 7)	0.70(15)	5.0
$5_{1,4} - 4_{1,3}$	101955.974	13.7	$9.18 \cdot 10^{-5}$	4.2(9)	5.20( 4)	0.38( 8)	10.4
<b>HNCOH<sup>+</sup></b>							
$5 - 4$	99559.525	14.3	$8.82 \cdot 10^{-6}$	<0.8			<3.3
<b>HNCO</b>							
$4_{0,4} - 3_{0,3}$ $F = 3 - 3$	87924.381	10.5	$7.25 \cdot 10^{-7}$	19(1)	5.33(1)	0.33(2)	53.5
$4_{0,4} - 3_{0,3}$ $F = 5 - 4$	87925.252	10.5	$9.02 \cdot 10^{-6}$	761(2)	5.31(1)	0.44(1)	1619.6
$4_{0,4} - 3_{0,3}$ $F = 4 - 3$	87925.252	10.5	$8.46 \cdot 10^{-6}$				
$4_{0,4} - 3_{0,3}$ $F = 3 - 2$	87925.252	10.5	$8.29 \cdot 10^{-6}$				
$4_{0,4} - 3_{0,3}$ $F = 4 - 4$	87925.898	10.5	$5.64 \cdot 10^{-7}$	24(1)	5.30(1)	0.40(2)	57.4
$5_{0,5} - 4_{0,4}$ $F = 4 - 4$	109904.922	15.8	$8.81 \cdot 10^{-7}$	12(1)	5.33(1)	0.34(3)	33.2
$5_{0,5} - 4_{0,4}$ $F = 6 - 5$	109905.758	15.8	$1.80 \cdot 10^{-5}$	553(1)	5.31(1)	0.36(1)	1450.3
$5_{0,5} - 4_{0,4}$ $F = 5 - 4$	109905.758	15.8	$1.73 \cdot 10^{-5}$				
$5_{0,5} - 4_{0,4}$ $F = 4 - 3$	109905.758	15.8	$1.71 \cdot 10^{-5}$				
$5_{0,5} - 4_{0,4}$ $F = 5 - 5$	109906.430	15.8	$7.21 \cdot 10^{-7}$	11(1)	5.31(2)	0.37(4)	28.2
<b>HOCN</b>							
$4_{0,4} - 3_{0,3}$	83900.569	10.1	$4.18 \cdot 10^{-5}$	50(1)	5.31(1)	0.47(1)	99.7
$5_{0,5} - 4_{0,4}$	104874.676	15.1	$8.36 \cdot 10^{-5}$	34(1)	5.30(1)	0.38(1)	83.2
<b>HCNO</b>							
$4 - 3$	91751.320	11.0	$3.84 \cdot 10^{-5}$	21(1)	5.33(1)	0.41(2)	47.4
$5 - 4$	114688.383	16.5	$7.67 \cdot 10^{-5}$	8(2)	5.35(3)	0.26(5)	28.6
<b>HONC</b>							
$4 - 3$	87625.193	10.5	$3.41 \cdot 10^{-5}$	<2.1			<8.1
$5 - 4$	109530.044	15.8	$6.81 \cdot 10^{-5}$	<1.6			<6.9

**Table A.2.** Formation enthalpy estimates in kcal mol<sup>-1</sup>

Species	$\Delta H$	Ref.
HNCO <sup>+</sup>	243	1
HOCN <sup>+</sup>	274	2
HCNO <sup>+</sup>	292	2
HONC <sup>+</sup>	331.7	2
HNOC <sup>+</sup>	331.4	2
H <sub>2</sub> NCO <sup>+</sup>	167	1
HNCOH <sup>+</sup>	183	3
HCNOH <sup>+</sup>	234.8	3
H <sub>2</sub> OCN <sup>+</sup>	240.9	3
H <sub>2</sub> CNO <sup>+</sup>	243	3

**Notes.** (1) Lias et al. (1984); (2) computed from Luna et al. (1996) using the experimental value for the most stable isomer HNCO<sup>+</sup>; (3) computed from Ijjaali et al. (2001) using the experimental value for the most stable isomer H<sub>2</sub>NCO<sup>+</sup>.

**Table A.3.** Assumed rate coefficients of the DR reaction of the CH<sub>2</sub>NO<sup>+</sup> ions.

Reaction	Rate Coefficient ( $\times 10^{-7}(T/300)^{-0.5} \text{ cm}^3 \text{ s}^{-1}$ )
H <sub>2</sub> NCO <sup>+</sup> + e → HNCO + H	2.50
H <sub>2</sub> NCO <sup>+</sup> + e → CO + NH <sub>2</sub>	0.50
H <sub>2</sub> NCO <sup>+</sup> + e → NCO + H <sub>2</sub>	1.50
H <sub>2</sub> CNO <sup>+</sup> + e → HCNO + H	2.50
H <sub>2</sub> CNO <sup>+</sup> + e → CH <sub>2</sub> + NO	0.50
HCNOH <sup>+</sup> + e → HCNO + H	2.50
HCNOH <sup>+</sup> + e → HONC + H	0.50
HCNOH <sup>+</sup> + e → HCN + OH	0.50
HNCOH <sup>+</sup> + e → HOCN + H	0.50
HNCOH <sup>+</sup> + e → HNCO + H	2.50
HNCOH <sup>+</sup> + e → HNC + OH	0.50
H <sub>2</sub> OCN <sup>+</sup> + e → HOCN + H	1.50
H <sub>2</sub> OCN <sup>+</sup> + e → H <sub>2</sub> O + CN	0.50